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Title: Introduction to Numerical Methods

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Introduction to Numerical Methods

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Numerical Methods

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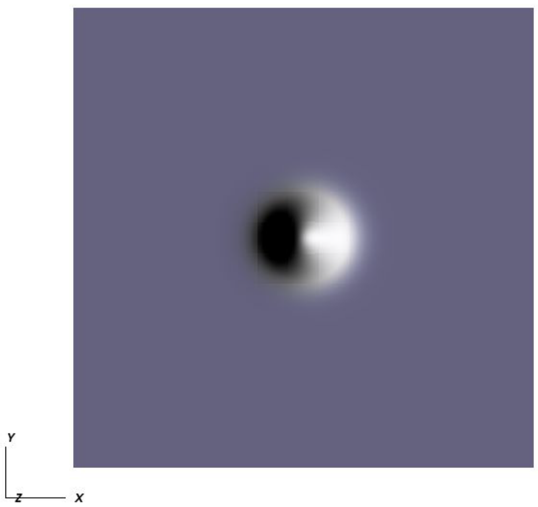
Repetitive algorithms to obtain approximate solutions to mathematical problems

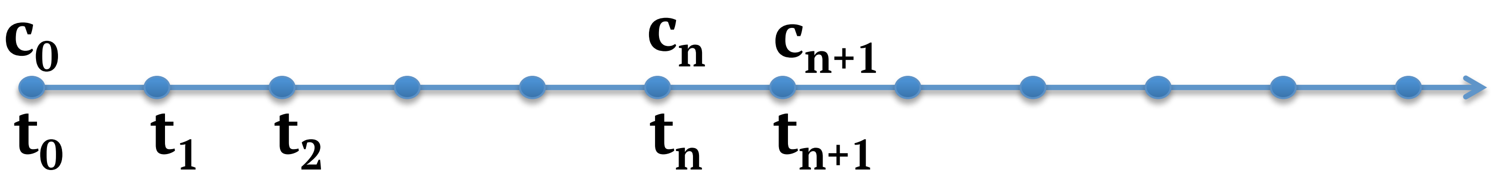


Sorting
Searching
Root Finding
Optimization
Interpolation
Extrapolation
Least squares regression
Eigenvalue Problems
Ordinary Differential Equations
Partial Differential Equations

Starting Simple

$$c_t = \lambda c$$

Goal : Given an initial condition, use basic arithmetic to estimate the solution at a later time.

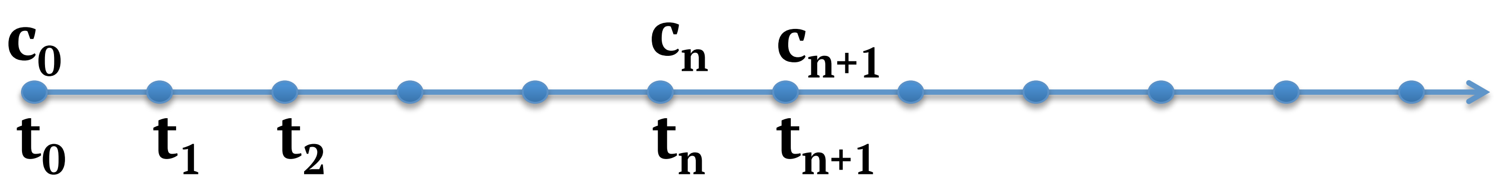


Continuous to Discrete

$$c_t = \lambda c$$

Use Taylor Series

$$c_t|_{t^n} = \frac{c^{n+1} - c^n}{\Delta t} + \frac{\Delta t}{2} c_{tt}|_{\xi}, \quad \xi \in [t_n, t^{n+1}]$$



Introducing Errors

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$$c^{n+1} = c^n + \lambda \Delta t c^n - \underbrace{\frac{\Delta t^2}{2} c_{tt}|_\xi}_{TruncationError}$$

Approximate the solution by dropping the truncation error

"Forward Euler"

$$\tilde{c}^{n+1} = \tilde{c}^n + \lambda \Delta t \tilde{c}^n$$

How big can the time step be ?

Time Step and Stability

How can we control the error growth ?

Error

$$E^n = c^n - \tilde{c}^n$$

$$E^{n+1} = \underbrace{(1 + \lambda \Delta t)}_{Amplification} \; E^n - \frac{\Delta t^2}{2} c_{tt}|_\xi$$

The truncation error acts as a source

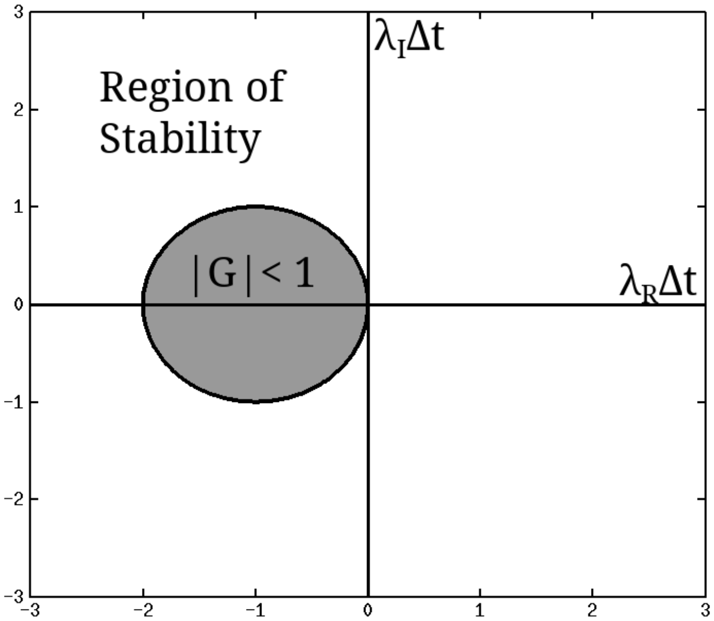
Error can be amplified!

Time Step and Stability

How can we control the error growth ?

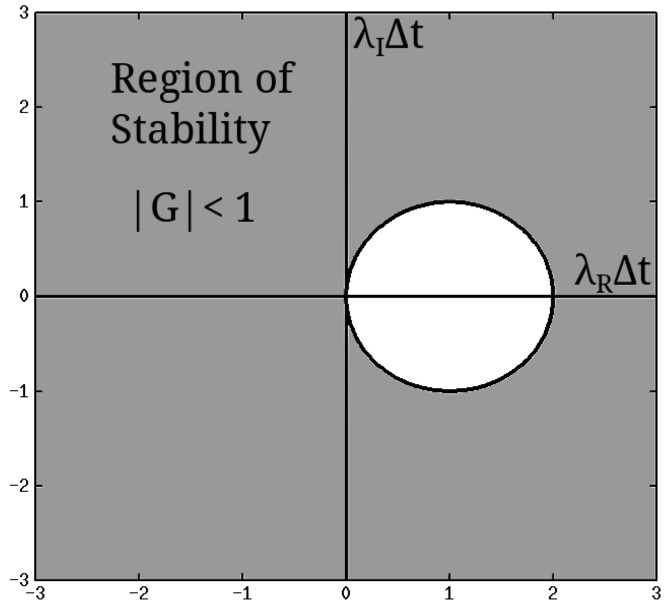
<u>Don't amplify the error!</u>

$$|G| = \left|\frac{\tilde{c}^{n+1}}{\tilde{c}^{n}}\right| = \underbrace{|1 + \lambda\Delta t|}_{ForwardEuler} < 1$$



Stability Diagrams and Implicit Integration Schemes

$$|G| = \underbrace{\left|\frac{1}{1-\lambda\Delta t}\right|}_{BackwardEuler} < 1$$



*Implicit schemes allow for larger time steps

Convergence

If the truncation error is $\mathcal{O}(\Delta t^n)$
and the integration scheme is stable,
then the approximate solution will converge
to the exact solution as $\Delta t \to 0$
at a rate proportional to Δt^n.

Systems of ODEs

PDE

$$\vec{s}_t + \nabla \cdot \vec{f} = \vec{q}$$

Spatial Discretization →

ODE System

$$\vec{c}_t = \boldsymbol{A}\vec{c}$$

Stability

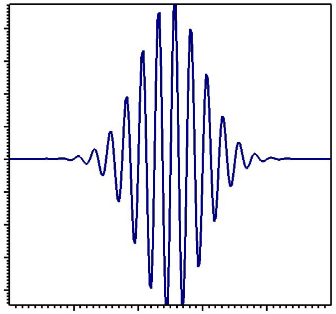
- Decoupling = Diagonalization

$$\boldsymbol{A} = \boldsymbol{P}\boldsymbol{D}\boldsymbol{P}^{-1}$$

- Maximum eigenvalue determines time step restrictions

$$(w_i)_t = \lambda_i w_i$$

Finite Difference Method
Upwind Advection



$$c_t + uc_x = 0$$

Use Taylor Series for the spatial derivative

Restrict the truncation to zero at each node

$$(\tilde{c}_i)_t = -\frac{u}{\Delta x}(\tilde{c}_i - \tilde{c}_{i-1})$$

Finite Difference Method

Upwind Advection

$$\vec{c}_t = \boldsymbol{A}\vec{c}$$

Spatial discretization results in a sparse ODE system;

$$A_{i,i} = \frac{-u}{\Delta x},\; A_{i,i-1} = \frac{u}{\Delta x}$$

Integration by Forward Euler

$$\tilde{c}_i^{n+1} = \tilde{c}_i^n - \frac{u\Delta t}{\Delta x}(\tilde{c}_i^n - \tilde{c}_{i-1}^n)$$

Finite Difference Method
Upwind Advection, Group Example

$$\tilde{c}_i^{n+1} = \tilde{c}_i^n - 0.5(\tilde{c}_i^n - \tilde{c}_{i-1}^n)$$

You each are assigned a process ID and three nodes

<u>To advance the system</u>

1. Exchange data with your "upstream neighbor"
2. Update the solution at your three nodes
3. Do your file I/O.
4. Wait for your neighbor to finish.
5. Repeat

Sample Solution Output

Solution.001.00000.data

i	c
1	0.000
2	0.000
3	0.000

Finite Difference Method

Implicit Upwind Advection

$$\tilde{c}_i^{n+1} = \tilde{c}_i^n - \frac{u\Delta t}{\Delta x}\underbrace{(\tilde{c}_i^{n+1} - \tilde{c}_{i-1}^{n+1})}_{\text{Evaluated at the next time step}}$$

Evaluated at the next time step

Forward Integration requires matrix inversion

$$(\boldsymbol{I} - \Delta t \boldsymbol{A})\vec{c}^{n+1} = \vec{c}^{n}$$

General Discretization Overview

- Approximate continuous functions by discrete observations
- Approximate derivative operators by difference operators

PDE

$$\vec{s}_t + \nabla \cdot \vec{f} = \vec{q}$$

Spatial Discretization →

ODE System

$$\vec{S}_t + \boldsymbol{A}\vec{S} = \vec{Q}$$

- Apply a suitable time integrator

Discretization Flavors

Mesh-based

Strong (Collocation)	Weak (Galerkin)	Conservative
Finite Difference	Finite Element	Finite Volume
Pseudo-Spectral	Spectral	
	Spectral Element	

Mesh-free

Smoothed Particle Hydrodynamics
Element-free Galerkin
Discrete Vortex Method
Radial Basis Methods

Stability and Work
Explicit Schemes

- Wall-Time ~ (Number of Floating Point Operations) /(FLOP/sec)
- Remember, stability requirements impose time-step restrictions

$$\lambda_{max}\Delta t < C$$

- We want to integrate to a known time, which requires M time-steps

$$M = \frac{T}{\Delta t}$$

- The number of floating point operations per time step is proportional to the number of degrees of freedom

$$W_{float} \propto \frac{NT\lambda(N)}{k_{FLOPS}}$$

Summary

- I showed too many equations.
- I am sorry.
- Discretizations
  - allow us to approximate solutions to mathematical models of physical systems using a repetitive algorithm.
  - introduce errors that can lead to numerical instabilities if we are not careful.
- We barely scratched the surface of numerical methods.
- Let's talk more!